

LIST OF REFERENCES CITED BY APPLICANT

(Use several sheets if necessary)

ATTY. DOCKET NO.

9476-003-999

APPLICATION NO.

09/644,937

APPLICANT

Nicholls

FILING DATE

August 23, 2000

GROUP

2887

1631

U.S. PATENT DOCUMENTS

*EXAMINER INITIAL		DOCUMENT NUMBER	DATE	NAME	CLASS	SUBCLASS	FILING DATE IF APPROPRIATE
AM	AA	4,855,931	08/08/89	Saunders	364	499	
	AB	5,025,388	06/18/91	Cramer, III et al.	364	496	
	AC	5,526,281	06/11/96	Chapman et al.	364	496	
	AD	5,703,792	12/30/97	Chapman	364	496	
	AE	6,070,127	05/30/00	Hirono et al.	702	27	
	AF	6,185,506	02/06/01	Cramer et al.	702	19	
AM	AG	6,240,374	05/29/01	Cramer et al.	703	11	

FOREIGN PATENT DOCUMENTS

		DOCUMENT NUMBER	DATE	COUNTRY	CLASS	SUBCLASS	TRANSLATION	
							YES	NO

OTHER REFERENCES (Including Author, Title, Date, Pertinent Pages, Etc.)

AM	AH	Apaya <i>et al.</i> , 1995, "The matching of electrostatic extrema: A useful method in drug design? A study of phosphodiesterase III inhibitors," <u>Journal of Computer-Aided Molecular Design</u> 9:33-43						
	AI	Arteca <i>et al.</i> , 1988, "Shape group studies of molecular similarity: relative shapes of Van der Waals and electrostatic potential surfaces of nicotinic agonists," <u>J. Mol. Graphics</u> 6:45-53						
	AJ	Artymiuk <i>et al.</i> , 1992, "Similarity searching in databases of three-dimensional molecules and macromolecules," <u>J. Chem. Inf. Comput. Sci.</u> 32(6):617-630						
	AK	Barros <i>et al.</i> , "Using the triangle inequality to reduce the number of comparisons required for similarity-based retrieval," <u>In: Proceedings of IS&T/SPIE: Storage and Retrieval for Still Image and Video Databases IV</u> , 28 Jan. - 2 Feb., 1996, Vol. 2670, pp. 392-403.						
	AL	Bath <i>et al.</i> , 1994, "Similarity searching in files of three-dimensional chemical structures: Comparison of fragment-based measures of shape similarity," <u>J. Chem. Inf. Comput. Sci.</u> 34:141-147						
	AM	Bradley <i>et al.</i> , 1993, "Deducing molecular similarity using voronoi binding sites," <u>J. Chem. Inf. Comput. Sci.</u> 33:750-755						
	AN	Carbo <i>et al.</i> , 1980, "How similar is a molecule to another? An electron density measure of similarity between two molecular structures," <u>International Journal of Quantum Chemistry XVII</u> :1185-1189						
	AO	Ciaccia <i>et al.</i> , "M-tree: An efficient access method for similarity search in metric spaces," <u>In: Proc. 23rd VLDB Conf.</u> , Jarke, M., Carey, M.J., Dittrich, K.R., Lochovsky, F.H., Loucopoulos, P., and Jeusfeld, M.A., eds., Athens, Greece, August 1997, pp. 426-435.						
	AP	Cioslowski and Nanyakkara, 1993, "Similarity of atoms in molecules," <u>J. Am. Chem. Soc.</u> 115:11213-11215						
	AQ	Clarkson, 1997, "Nearest neighbor queries in metric spaces," <u>Proc. 29th ACM Symp. Theory Comp.</u> , pp. 609-617.						
AM	AR	Constans <i>et al.</i> , 1997, "Toward a global maximization of the molecular similarity function: Superposition of two molecules," <u>J. Comput. Chem.</u> 18(6):826-846						

AM	AS	Cramer, III <i>et al.</i> , 1974, "Substructural analysis. A novel approach to the problem of drug design," <u>Journal of Medicinal Chemistry</u> 17 (5):533-535
	AT	Doman <i>et al.</i> , 1996, "Algorithm5: A technique for fuzzy similarity clustering of chemical inventories," <u>J. Chem. Inf. Comput. Sci.</u> 36 (6):1195-1204
	AU	Drefahl and Reinhard, 1993, "Similarity-based search and evaluation of environmentally relevant properties for organic compounds in combination with the group contribution approach," <u>J. Chem. Inf. Comput. Sci.</u> 33 (6):886-895
	AV	Dughan <i>et al.</i> , 1991, "The study of peptide bond isosteres using molecular similarity," <u>Journal of Molecular Structure (Theochem)</u> 235 :481-488
	AW	Feustel and Shapiro, 1982, "The nearest neighbor problem in an abstract metric space," <i>In: Pattern Recognition Letters</i> 1 :125-128.
	AX	Good <i>et al.</i> , 1992, "Utilization of Gaussian functions for the rapid evaluation of molecular similarity," <u>J. Chem. Inf. Comput. Sci.</u> 32 (3):188-191
	AY	Good <i>et al.</i> , 1992, "Similarity screening of molecular data sets," <u>Journal of Computer-Aided Molecular Design</u> 6 :513-520
	AZ	Good <i>et al.</i> , 1995, "New molecular shape descriptors: Application in database screening," <u>Journal of Computer-Aided Molecular Design</u> 9 :1-12
	BA	Grant <i>et al.</i> , 1996, "A fast method of molecular shape comparison: A simple application of a Gaussian description of Molecular Shape," <u>Journal of Computational Chemistry</u> 17 (14):1653-66
	BB	Greene <i>et al.</i> , 1994, "Chemical Function Queries for 3D Database Search," <u>J. Chem. Inf. Comput. Sci.</u> 34 :1297-1308
	BC	Grethe and Hounshell, "Similarity Searching in the development of new bioactive compounds . An application," <i>In: Chemical Structures 2</i> , Warr, W. A., ed., Springer-Verlag, Heidelberg. 1993. Pages 399-407.
	BD	Hahn, 1997, "Three-dimensional shape-based searching of conformationally flexible compounds," <u>J. Chem. Inf. Comput. Sci.</u> 37 (1):80-86
	BE	Hodgkin and Richards, 1987, "Molecular similarity based on electrostatic potential and electric field," <u>International Journal of Quantum Chemistry: Quantum Biology Symposium</u> 14 :105-110
	BF	Hudson <i>et al.</i> , 1996, "Parameter based methods for compound selection from chemical databases," <u>Quant. Struct.-Act. Relat.</u> 15 :285-289
	BG	Jain <i>et al.</i> , 1994, "Compass: Predicting biological activities from molecular surface properties. Performance comparisons on a steroid benchmark," <u>Journal of Medicinal Chemistry</u> 37 (15):2315-2327
	BH	Johnson, 1989, "A review and examination of the mathematical spaces underlying molecular similarity analysis," <u>Journal of Mathematical Chemistry</u> 3 :117-145
	BI	Kato <i>et al.</i> , 1987, "A novel method for superimposing molecules and receptor mapping," <u>Tetrahedron</u> 43 (22):5229-5236
	BJ	Martin <i>et al.</i> , 1990, "Searching databases of three-dimensional structures," <i>In: Reviews of Computational Chemistry</i> , Kipkowitz, K. and Boyd, D.B., eds., Vol. 1, pp. 213-263.
	BK	Mestres <i>et al.</i> , 1997, "MIMIC: A molecular-field matching program. Exploiting applicability of molecular similarity approaches," <u>J. Comput. Chem.</u> 18 (7):934-954
	BL	Meyer and Richards, 1991, "Similarity of molecular shape," <u>Journal of Computer-Aided Molecular Design</u> 5 :427-439
	BM	Mezey, 1987, "The shape of molecular charge distributions: group theory without symmetry," <u>Journal of Computational Chemistry</u> 8 (4):462-469
AM	BN	Mezey, 1992, "Shape-similarity measures for molecular bodies: A three-dimensional topological approach to quantitative shape-activity relations," <u>J. Chem. Inf. Comput. Sci.</u> 32 (6):650-656

AM	BO	Perry and van Geerestein, 1992, "Database searching on the basis of three-dimensional molecular similarity using the SPERM program," <u>J. Chem. Inf. Comput. Sci.</u> 32 (6):607-616
	BP	Petitjean, 1995, "Geometric molecular similarity from volume-based distance minimization: Application to saxitoxin and tetrodotoxin," <u>Journal of Computational Chemistry</u> 16 (1):80-90
	BQ	Petitjean, 1996, "Three-dimensional pattern recognition from molecular distance minimization," <u>J. Chem. Inf. Comput. Sci.</u> 36 (5):1038-1049
	BR	Petke, 1993, "Cumulative and discrete similarity analysis of electrostatic potentials and fields," <u>Journal of Computational Chemistry</u> 14 (8):928-933
	BS	Reynolds <i>et al.</i> , 1998, "Lead discovery using stochastic cluster analysis (SCA): A new method for clustering structurally similar compounds," <u>J. Chem. Inf. Comput. Sci.</u> 38 (2):305-312
	BT	Richard, 1991, "Quantitative comparison of molecular electrostatic potentials for structure-activity studies," <u>Journal of Computational Chemistry</u> 12 (8):959-969
	BU	Sprague and Hoffman, "CATALYST Pharmacophore models and their utility as queries for searching 3D databases," <i>In: Computer Assisted Lead Finding and Optimization: Current Tools for Medicinal Chemistry</i> , Van de Waterbeemd, H., Testa, B., Folkers, G., eds., VCHA-Basel, 1997, pp. 223-240
	BV	Thorner <i>et al.</i> , 1997, "Similarity searching in files of three-dimensional chemical structures: Representation and searching of molecular electrostatic potentials using field-graphs," <u>Journal of Computer-Aided Molecular Design</u> 11 :163-174
	BW	Uhlmann, 1991, "Satisfying general proximity/similarity queries with metric trees," <i>In: Information Processing Letters</i> 40 (4):175-179.
	BX	Walker <i>et al.</i> , 1993, "Shape groups of the electronic isodensity surfaces for small molecules: shapes of 10-electron hydrides," <u>Journal of Computational Chemistry</u> 14 (10):1172-1183
AM	BY	Weiser <i>et al.</i> , 1999, "Optimization of Gaussian surface calculations and extension to solvent-accessible surface areas," <u>Journal of Computational Chemistry</u> 20 (7):688-703
EXAMINER		DATE CONSIDERED
Andi Marscher		9-6-02
<p>*EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609; Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to applicant.</p>		